

IN THE CLAIMS:

The text of all pending claims, (including withdrawn claims) is set forth below. Cancelled and not entered claims are indicated with claim number and status only. The claims as listed below show added text with underlining and deleted text with ~~strikethrough~~. When strikethrough cannot easily be perceived, or when five or fewer characters are deleted, [[double brackets]] are used to show the deletion. The status of each claim is indicated with one of (original), (currently amended), (cancelled), (withdrawn), (new), (previously presented), or (not entered).

Please AMEND claims 13 and 24 in accordance with the following:

1. – 12. (cancelled)

13. (currently amended) A method of analyzing, by a computer processor, three-dimensional structures of sequences of atoms or atomic groups of molecules of substances, including a first structure of a sequence of atoms or an atomic group of a molecule of a first substance expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure of a sequence of atoms or an atomic group of a molecule of a second substance expressed by three-dimensional coordinates of elements belonging to a second point set, comprising:

dividing the second point set into a plurality of subsets each having a size that is determined by the size of the first point set;

generating a combination of correspondence satisfying a restriction condition between the elements belonging to the first point set and the elements belonging to each of the subsets of the second point set from among all candidates for the combination of correspondence; and

calculating a root mean square distance between the elements corresponding in the combination of correspondence generated, and

wherein the restriction condition includes a condition such that an attribute value of each of the elements belonging to the first point set coincides with an attribute value of the corresponding element belonging to the second point set in a candidate for combination of correspondence,

determining if a degree of spatial similarity between the first structure of the sequence of atoms or the atomic group of the molecule of the first substance and the second structure of the sequence of atoms or the atomic group of the molecule of the second substance is greater than or equal to a predetermined threshold degree of similarity; and

outputting a determination, if the degree of spatial similarity between the first structure of the sequence of atoms or the atomic group of the molecule of the first substance

and the second structure of the sequence of atoms or the atomic group of the molecule of the second substance is greater than or equal to the predetermined threshold degree of similarity, that a function of the first structure of the sequence of atoms or the atomic group of the molecule of the first substance is substantially equivalent to a function of the second structure of the sequence of atoms or the atomic group of the molecule of the second substance.

14. (previously presented) The method of claim 13, wherein the second point set is divided into the subsets so that the number of elements belonging to each of the subsets is a function of the number of elements belonging to the first point set.

15. (previously presented) The method of claim 13, wherein the second point set is divided into the subsets so that a spatial size of each of the subsets is nearly equal to a spatial size of the first point set.

16. – 23. (cancelled)

24. (currently amended) A method of analyzing, by a computer, three-dimensional structures of sequences of atoms or atomic groups of molecules of substances including a first structure of a sequence of atoms or an atomic group of a molecule of a first substance expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure of a sequence of atoms or an atomic group of a molecule of a second substance expressed by three-dimensional coordinates of elements belonging to a second point set, comprising:

dividing the second point set into a plurality of subsets each having a size that is determined by the size of the first point set;

generating a combination of correspondence such that an attribute value of each of the elements belonging to the first point set coincides with an attribute value of the corresponding element belonging to the each of the subsets of the second point set from among all candidates for the combination of correspondence;

calculating a root mean square distance (rmsd) between the elements corresponding in the combination of correspondence generated, and

where the rmsd is less than a predetermined threshold value, determining that the elements of the first point set coincide with or are similar to the subset of the second point set corresponding in the combination of correspondence generated and storing a correspondence/~~similarity~~similarity determination on a computer readable recording medium,
determining if a degree of spatial similarity between the first structure of the

sequence of atoms or the atomic group of the molecule of the first substance and the second structure of the sequence of atoms or the atomic group of the molecule of the second substance is greater than or equal to a predetermined threshold degree of similarity; and

outputting a determination, if the degree of spatial similarity between the first structure of the sequence of atoms or the atomic group of the molecule of the first substance and the second structure of the sequence of atoms or the atomic group of the molecule of the second substance is greater than or equal to the predetermined threshold degree of similarity, that a function of the first structure of the sequence of atoms or the atomic group of the molecule of the first substance is substantially equivalent to a function of the second structure of the sequence of atoms or the atomic group of the molecule of the second substance.

25. (previously presented) The method of claim 24, wherein the second point set is divided into the subsets so that the number of elements belonging to each of the subsets is a function of the number of elements belonging to the first point set.

26. (previously presented) The method of claim 24, wherein the second point set is divided into the subsets so that a spatial size of each of the subsets is nearly equal to a spatial size of the first point set.